

Quantum Simulation of Markov Chains

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Abstract. The possibility of simulating a stochastic process by the intrinsic randomness of quantum system is investigated. Two simulations of Markov Chains by the measurements of quantum systems are proposed.

1 Introduction

Stochastic simulation methods, also commonly known as Monte Carlo methods, are important in scientific computing. Such methods are useful for studying deterministic problems that are too complicated to model analytically or deterministic problems whose high dimensionality makes standard discretizations infeasible. Stochastic simulations [1] are usually realized by classical computer algorithms, which are actually deterministic. In this paper, we study the possibility of simulating a stochastic process by the intrinsic randomness of quantum system. We believe that, theoretically speaking, a quantum system may simulate a stochastic process better than a classical system due to its intrinsic randomness.

Markov Chain is a basic and widely studied stochastic process. It is also useful in scientific computing. For example, one can solve partial differential equations or groups of linear equations by simulations of Markov Chains. In this paper we will propose two simulations of Markov Chains by the measurements of quantum systems. The second simulation is closely related to the reading of a quantum register and thus may be realized by quantum computer. It thus seems that quantum computer might be a better choice than classical computer for carrying out Monte Carlo method.

2 Definition of Markov Chain

In probability theory, the concept of experiment occupies a crucial position. Roughly speaking, an experiment consists of a space of its possible outcomes, together with an assignment of probabilities to each of these outcomes. In this paper, we only consider experiments with finitely many outcomes. Let I be a finite set. The formal definition of an experiment (with finitely many outcomes) is as follows[2].

Definition 1. A function $\lambda : I \rightarrow [0, 1]$ is called a distribution on I if $\sum_{i \in I} \lambda(i) = 1$. When λ is a distribution on I it will be denoted by $\lambda = (\lambda_i : i \in I)$ where $\lambda_i = \lambda(i)$.

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Definition 2. An experiment E is a pair (Ω, p) where $\Omega = \{\omega_i | i \in I\}$ is a finite set of the outcomes of E , called the sample space of E , and $p = (p_i : i \in I)$ is a distribution on I , called the distribution of E , where $p_i = p(\omega_i)$.

Another ingredient necessary for the definition of Markov Chain is the concept of stochastic matrix.

Definition 3. A matrix $P = (p_{ij})_{i,j \in I}$ is called stochastic if for each $i \in I$ $p^i = (p_{ij} : j \in I)$ is a distribution on I .

Now let us introduce the definition of Markov Chain.

Definition 4. Let $P = (p_{ij})_{i,j \in I}$ be a stochastic matrix. A (finite or infinite sequence) of experiments $(E_n)_{n \geq 0}$ is called a Markov Chain with the transition matrix P if all the experiments in the sequence have the same sample space $\Omega = \{\omega_i | i \in I\}$ and for each $n \geq 0$ the distribution of the experiment E_{n+1} only depends on the outcome of the experiment E_n in the following way: when the outcome of E_n is ω_i the distribution of E_{n+1} is $p^i = (p_{ij} : j \in I)$.

From probability point of view, the behavior of a Markov Chain $(E_n)_{n \geq 0}$ is completely determined by its transition matrix and its initial distribution, namely, the distribution of the experiment E_0 .

Remark. The above definition of Markov Chain might not be formal or rigorous enough from mathematical point of view. But for our modest purpose in this paper Definition 4 is adequate. For the definition of Markov Chain based on the terminology of probability space and conditional probability [3], which is mathematically beyond question, the reader who has a passion for mathematical rigor and precision can refer to mathematical text books on probability theory.

3 Simulation of Markov Chains by Angular Momentum System

In this section we will propose a realization of Markov Chains by a sequence of quantum measurements for angular momenta.

Consider a spin s system \mathbb{S} . Let \hat{S}_x , \hat{S}_y and \hat{S}_z be the x , y and z components of the spin operator $\hat{\mathbf{S}}$ of \mathbb{S} .

Let R be the operator of a rotation through an angle θ about a direction specified by the unit vector \mathbf{n} . Then we have $R = e^{-i\theta\mathbf{n}\cdot\hat{\mathbf{S}}}$, which is clearly unitary. Suppose that this rotation is specified by the Eulerian angles (α, β, γ) , then by definition it can be carried out in three stages: (1) a rotation through the angle α ($0 \leq \alpha \leq 2\pi$) about the z -axis, (2) a rotation through the angle β ($0 \leq \beta \leq \pi$) about the new position y' of the y -axis, (3) a rotation through the angle γ ($0 \leq \gamma \leq 2\pi$) about the resulting final position z'' of the z -axis. Correspondingly, we have

$$R = e^{-i\theta\mathbf{n}\cdot\hat{\mathbf{S}}} = e^{-i\gamma\hat{S}_{z''}}e^{-i\beta\hat{S}_{y'}}e^{-i\alpha\hat{S}_z} = e^{-i\alpha\hat{S}_z}e^{-i\beta\hat{S}_y}e^{-i\gamma\hat{S}_z}.$$

Now define $\hat{S}_{\mathbf{n}} = R^\dagger \hat{S}_z R$. Physically, it represents the component of the spin operator $\hat{\mathbf{S}}$ in the direction specified by the vector \mathbf{n} . Let $\{|sm\rangle|m =$

$s, s-1, \dots, -s\}$ be the state vectors of the spin system \mathbb{S} that span the standard $2s+1$ dimensional irreducible representation space of the Lie algebra generated by the spin operators \hat{S}_x , \hat{S}_y and \hat{S}_z . To be precise, we have

$$\hat{\mathbf{S}}^2|sm\rangle = s(s+1)|sm\rangle, \quad \hat{S}_z|sm\rangle = m|sm\rangle.$$

Let $|sm'\rangle = R^{-1}|sm\rangle$ for each m . Then we have

$$\langle sm'_2|sm_1\rangle = \langle sm_2|e^{-i\alpha\hat{S}_z}e^{-i\beta\hat{S}_y}e^{-i\gamma\hat{S}_z}|sm_1\rangle = e^{-im_2\alpha}\langle sm_2|e^{-i\beta\hat{S}_y}|sm_1\rangle e^{-im_1\gamma}.$$

Denoting this quantity by $D_{m_2m_1}^s(\alpha, \beta, \gamma)$, we have

$$D_{m_2m_1}^s(\alpha, \beta, \gamma) = e^{-im_2\alpha}d_{m_2m_1}^s(\beta)e^{-im_1\gamma},$$

where

$$d_{m_2m_1}^s(\beta) = \langle sm_2|e^{-i\beta\hat{S}_y}|sm_1\rangle.$$

Similarly, it is easy to check that

$$\langle sm_2|sm'_1\rangle = \overline{D_{m_1m_2}^s(\alpha, \beta, \gamma)} = e^{im_1\alpha}\overline{d_{m_1m_2}^s(\beta)}e^{im_2\gamma},$$

where the “overline” means taking complex conjugation. But it can be proved that

$$\overline{d_{m_1m_2}^s(\beta)} = d_{m_1m_2}^s(\beta) = (-)^{m_1-m_2}d_{m_2m_1}^s(\beta),$$

it thus follows that

$$|\langle sm'_2|sm_1\rangle|^2 = |\langle sm_2|sm'_1\rangle|^2 = |d_{m_2m_1}^s(\beta)|^2.$$

Notice that when the system \mathbb{S} is in the state $|sm'\rangle$ and a measurement of S_z is carried out then $|\langle sm_2|sm'_1\rangle|^2$ is exactly the probability that the measurement will give the value m_2 . Likewise, when the system \mathbb{S} is in the state $|sm\rangle$ and a measurement of $S_{\mathbf{n}}$ is carried out then $|\langle sm'_2|sm_1\rangle|^2$ is exactly the probability that the measurement will give the value m_2 . That these two probabilities are identical, as shown above, prompts us to propose the following realization of Markov Chains by the proper measurements on the system \mathbb{S} .

Denote by M and M' respectively the measurements of S_z and $S_{\mathbf{n}}$ on the system \mathbb{S} . Let us consider the sequence $(M_n)_{n \geq 0}$ of measurements, where M_n stands for M when n is even and stands for M' when n is odd. We observe that each M_n can naturally be regarded as an experiment in the sense of Definition 2, with the sample space $\Omega = \{s, s-1, \dots, -s\} \triangleq I$, which is independent of n . On the other hand, the distribution of M_{n+1} only depends on the outcome of M_n in the following way: when the outcome of M_n is m_1 , the distribution of M_{n+1} is $p^{m_1} = (|d_{m_2m_1}^s(\beta)|^2 : m_2 \in I)$. The reason is, if the measurement M or M' gives the value m_1 , then the system will collapse to the state $|sm_1\rangle$ or $|sm'_1\rangle$ after the measurement.

Now it should be clear that the above defined the sequence $(M_n)_{n \geq 0}$ of measurements can be regarded as a simulation of the Markov Chain with the

transition matrix $(p_{ij})_{i,j \in I}$ where $p_{ij} = |d_{ji}^s(\beta)|^2$. If the system \mathbb{S} is initially in the state $|\psi\rangle$, then this Markov Chain has the initial distribution $\{\langle sm|\psi\rangle|^2 : m \in I\}$.

An interesting case arise when we take $s = 1/2$, $\beta = \pi/2$ and $\alpha = \gamma = 0$. In this case $\hat{\mathbf{S}}_n = \hat{S}_x$ and the sample space of M_n is $\{1/2, -1/2\}$. Moreover, we have

$$|d_{m_2 m_1}^{1/2}(\pi/2)|^2 = 1/2, \forall m_1, m_2 \in \{1/2, -1/2\}.$$

Thus the sequence $(M_n)_{n \geq 0}$ can be regarded as a simulation of the coin tossing experiment and the system \mathbb{S} may be used as a random numbers generator.

4 Simulation of Markov Chains by q-Bit System

Essentially based on the idea of the last section we propose in this section a simulation of Markov Chains by q-bit system.

We model a q-bit as a spin 1/2 system \mathbb{S} and keep the same notation for the system \mathbb{S} as in the last section. Let us consider the q-bit system \mathbb{Q}_N that is composed of N independent q-bits. Denote by $\hat{\mathbf{S}}^i$ the angular momentum operator of the i th q-bit and by $\hat{\mathbf{J}}$ the angular momentum operator of the q-bit system \mathbb{Q}_N . As in the last section we define $\hat{J}_{\mathbf{n}} = R^\dagger \hat{J}_z R$. By definition we have

$$\hat{\mathbf{J}} = \sum_{i=1}^N \hat{\mathbf{S}}^i, \quad \hat{J}_{\mathbf{n}} = \sum_{i=1}^N \hat{S}_{\mathbf{n}}^i.$$

Now consider the measurement of J_z carried out by measuring each S_z^i and the measurement of $J_{\mathbf{n}}$ carried out by measuring each $S_{\mathbf{n}}^i$. We denote these two kinds of measurement by M and M' respectively.

For convenience, we introduce the state vectors $|+\rangle$, $|-\rangle$, $|+_{\mathbf{n}}\rangle$ and $|-_n\rangle$ as follows:

$$S_z|+\rangle = \frac{1}{2}|+\rangle, S_z|-\rangle = -\frac{1}{2}|-\rangle, S_{\mathbf{n}}|+_{\mathbf{n}}\rangle = \frac{1}{2}|+_{\mathbf{n}}\rangle, S_{\mathbf{n}}|-_n\rangle = -\frac{1}{2}|-_n\rangle.$$

Then, from the general formula for the matrix element $d_{m_2 m_1}^s(\beta)$ we have

$$|\langle +_{\mathbf{n}}|+\rangle|^2 = |\langle +|+_{\mathbf{n}}\rangle|^2 = |\cos \beta/2|^2, \quad |\langle -_{\mathbf{n}}|+\rangle|^2 = |\langle -|+_{\mathbf{n}}\rangle|^2 = |\sin \beta/2|^2$$

and

$$|\langle +_{\mathbf{n}}|-\rangle|^2 = |\langle +|-_{\mathbf{n}}\rangle|^2 = |\sin \beta/2|^2, \quad |\langle -_{\mathbf{n}}|-\rangle|^2 = |\langle -|-_{\mathbf{n}}\rangle|^2 = |\cos \beta/2|^2.$$

According to the theory of quantum measurement, after the measurement M each q-bit is either in the state $|+\rangle$ or in the state $|-\rangle$ and after the measurement M' each q-bit is either in the state $|+_{\mathbf{n}}\rangle$ or in the state $|-_n\rangle$. Thus, after the measurement M , if its outcome is j , then $N/2 + j$ q-bits of the system \mathbb{Q}_N collapse to the state $|+\rangle$ and the other $N/2 - j$ q-bits collapse to the state $|-\rangle$.

Denote by $q_{j'j}$ the probability that the measurement M' on the system \mathbb{Q}_N which has just experienced the measurement M that gives the value j , will give the value j' . It then follows that if $j \geq j'$

$$q_{j'j} = \sum_{m=j-j'}^{N/2-j'} \binom{N/2+j}{m} \binom{N/2-j}{N/2-j'-m} |\cos \beta/2|^{2(N+j-j'-2m)} |\sin \beta/2|^{2(j'-j+2m)}$$

and if $j \leq j'$

$$q_{j'j} = \sum_{m=j'-j}^{N/2+j'} \binom{N/2-j}{m} \binom{N/2+j}{N/2+j'-m} |\cos \beta/2|^{2(N-j+j'-2m)} |\sin \beta/2|^{2(j-j'+2m)}.$$

Moreover, it is easily check that $q_{j'j}$ is also the probability that the measurement M on the system \mathbb{Q}_N which has just experienced the measurement M' that gives the value j , will give the value j' . It should then be clear that the sequence $(M_n)_{n \geq 0}$ of measurements, where M_n stands for M when n is even and stands for M' when n is odd, can be regarded as a simulation of the Markov Chain with the transition matrix $(q_{j'j})_{-N/2 \leq j', j \leq N/2}$.

References

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